GROMACS - Bug #961

SHAKE errors are reported incorrectly and may occasionally go unnoticed

06/21/2012 04:54 PM - Erik Marklund

Status: Closed
Priority: Normal
Assignee: David van der Spoel
Category: mdrun
Target version: 4.5.6
Affected version - extra info:

Description

A) vec_shakef() calls cshake() and inspects the variable "error" to see if the constraints were applied successfully. error is supposed to hold the index in an array of constraints, so by looking at error one knows which constraint that caused the problem. This is problematic, since if the first constraint in the array (index 0) was unsuccessfully applied then error is 0 and everything looks ok:

```c
error=0;
nconv=1;
for(nit=0; (nit<maxnit) && (nconv != 0) && (error == 0); nit++) {
    nconv=0;
    for(ll=0; (ll<ncon) && (error == 0); ll++) {
        < snip >
        if (rrpr < toler*mytol)
            error=ll;
        < snip >
    }
}
```

As seen, ll and error can be 0 when something goes wrong.

B) When there's a SHAKE error the atoms and the constraint are not reported correctly to stderr. Currently we have the following:

```c
else if (error != 0) {
    < snip >
    fprintf(stderr,"Inner product between old and new vector <= 0.0!\n"
            "constraint #%d atoms %u and %u\n",
            error-1,iatom[3*(error-1)+1]+1,iatom[3*(error-1)+2]+1);
    nit=0;
}
```

We report that constraint nr error-1 was bad, which is nonsense. Especially in the case where the first constraint was to blame. Consequently, we also report that atoms belonging to that wrongfully accused constraint are part of the problem.

SUGGESTED REMEDY: set error to the constraint index+1 in cshake() and crattle().

Associated revisions

Revision 7c611bab - 06/21/2012 06:14 PM - David van der Spoel
Fixes #961 - Shake reports wrong error

The constraint index reported by shake was off by 1.

Change-Id: I6f4d0c013b30f5963fb312b41fb87e90e6314619
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Change-Id: l6f4d0c013b30f5963fb312b41fb87e90e6314619

History
#1 - 06/21/2012 04:58 PM - Erik Marklund
- Assignee changed from Berk Hess to David van der Spoel

First of all, sorry for the formatting in the initial post. It was unintentional.
Secondly, I didn't mean to assign it to Berk. I changed the assignee to David, but I could also fix this myself if David's not up for it.

#2 - 06/22/2012 06:55 AM - David van der Spoel
- Status changed from New to Closed

Fixed in commit https://gerrit.gromacs.org/#q,I6f4d0c013b30f5963fb312b41fb87e90e6314619.n.z.